Glutaric acid, di(2,4,4-trimethylpentyl) ester

Inchi: InChI=1S/C21H40O4/c1-16(12-20(3,4)5)14-24-18(22)10-9-11-19(23)25-15-17(2)13-21(6
InchiKey: ARWFUUWYTHXGTH-UHFFFAOYSA-N
Formula: C21H40O4
SMILES: CC(COC(=O)CCCC(=O)OCC(C)CC(C)(C)C)CC(C)(C)C
Mol. weight [g/mol]: 356.54

Physical Properties

Property code	Value	Unit	Source
gf	-341.10	kJ/mol	Joback Method
hf	-994.43	kJ/mol	Joback Method
hfus	33.85	kJ/mol	Joback Method
hvap	77.28	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	5.388		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
rinpol	2229.00		NIST Webbook
tb	825.12	K	Joback Method
tc	1018.48	K	Joback Method
tf	445.59	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.76	J/mol×K	825.12	Joback Method
cpg	1051.59	J/mol×K	857.35	Joback Method
cpg	1069.27	J/mol×K	889.57	Joback Method
cpg	1085.85	J/mol×K	921.80	Joback Method
cpg	1101.37	J/mol×K	954.03	Joback Method
cpg	1115.89	J/mol×K	986.25	Joback Method
cpg	1129.45	J/mol×K	1018.48	Joback Method
dvisc	0.0009900	Pa×s	445.59	Joback Method
dvisc	0.0003645	Pa×s	508.85	Joback Method

dvisc	0.0001674	Pa×s	572.10	Joback Method
dvisc	0.0000898	Pa×s	635.36	Joback Method
dvisc	0.0000539	Pa×s	698.61	Joback Method
dvisc	0.0000352	Pa×s	761.87	Joback Method
dvisc	0.0000246	Pa×s	825.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377240&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume